MULTISCALE MODELING AND HOMOGENIZATION OF STRESSED GRAIN GROWTH

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The process of grain growth involves moving interfaces and topological changes of grain boundary geometry, and this cannot be effectively modeled by the Lagrangian, Eulerian, or Arbitrary Lagrangian Eulerian finite element method when stress effect is considered. In this work, we first introduce a variational equation based on the balance of energies associated with grain boundary surface tension and curvature, elastic strain energy, and the elastic strain energy difference due to anisotropy between adjacent grains. This reflects the coupling of elastic deformation of grains with grain boundary migration and thus necessitates the discretization of grain boundaries and grain domains. Using finite element method to study the migration of grain boundaries leads to a severe mesh distortion in each grain, and the topological changes of grain structures further demand a complete remeshing. To address these issues, a double-grid method is introduced. The elastic deformation of grains is discretized by a meshfree reproducing kernel approximation with built-in strain discontinuities along the grain boundaries, whereas the grain boundary migration kinematics is discretized using the standard finite element approximation. A brief overview of meshfree method will also be given.

The macroscopic mechanical, thermal, and electromagnetic properties of materials are essentially determined by the microstructures of materials. Such an understanding can be achieved neither by continuum analysis that completely ignores the microstructure, heterogeneity, or defects of materials, nor by atomic level simulations that have inherent time and length-scale limitations. The multi-scale mathematical and computational framework for bridging the physics of different scales is of critical importance to materials modeling. The second part of this presentation will discuss a preliminary study on multiscale homogenization and localization using an asymptotic expansion method and a wavelet based multiresolution analysis for modeling of heterogeneous materials.

[1] J. S. Chen, H. Lu, D. Moldovan, and D. Wolf, "A Double-Grid Method for Modeling of Microstructure Evolution," The 5th World Congress on Computational Mechanics, Proceeding, Vienna, Austria, July 7-12, 2002.

[2] J. S. Chen, C. Pan, C. T. Wu, and W. K. Liu, Reproducing Kernel Particle Methods for Large Deformation Analysis of Nonlinear Structures*, Computer Methods in Applied Mechanics and Engineering*, 139, 195-227, 1996.

[3] D. Moldovan, D. Wolf, S. R. Phillpot , and A. J. Haslam, *Philosophical Magazine* A, 82, 1271-1297, 2002.

[4] M. Brewster and G. Beylkin, "A Multiresolution Strategy for Numerical Homogenization", *Appl. Comput. Harmon. Anal.*, 2, pp. 327-349, 1995.